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FACULTY OF ENGINEERING AND ARCHITECTURE

Evaluation of Cu based catalysts for glycerol hydrogenolysis

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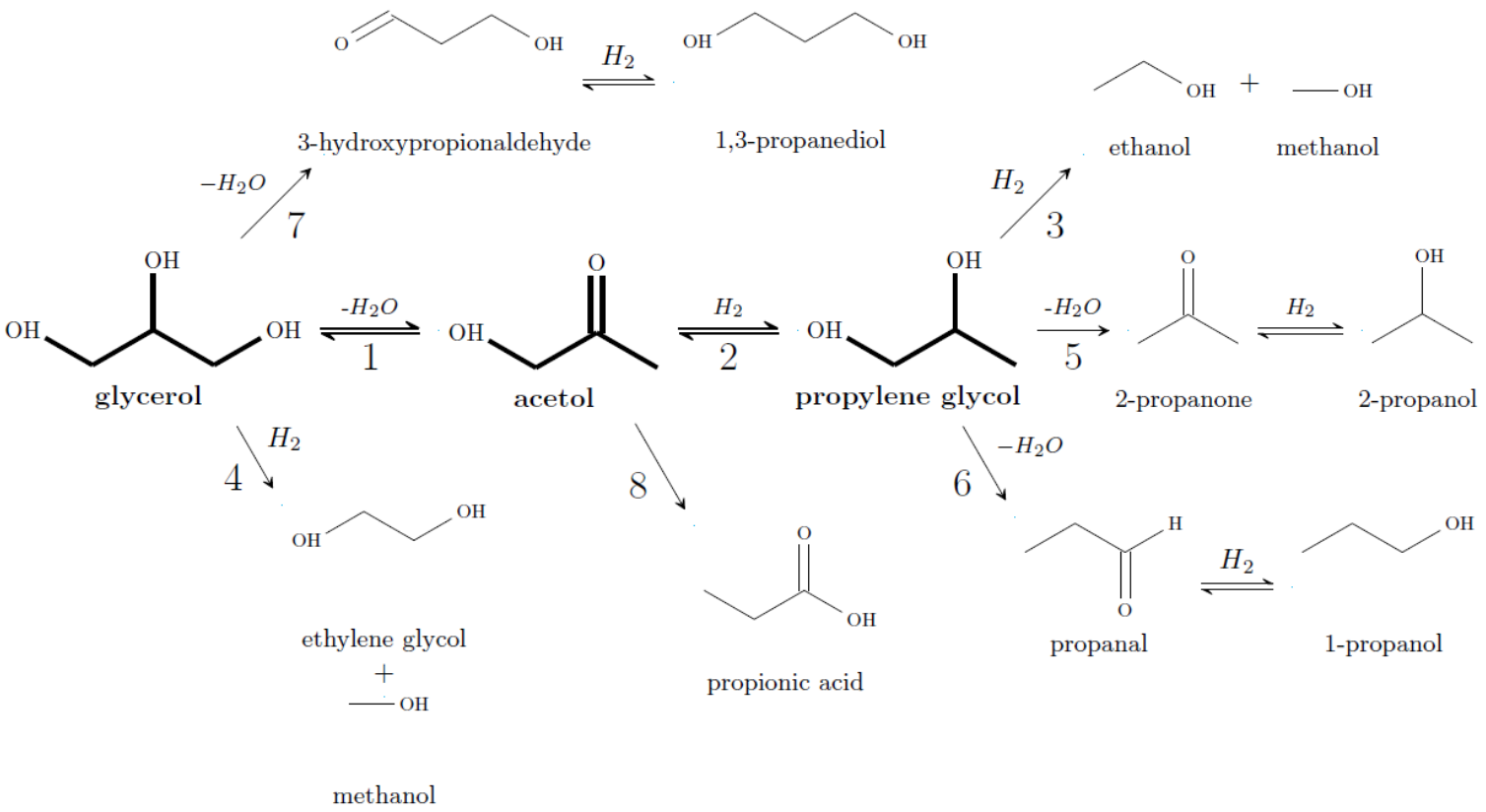
MCR-X, Svetlogorsk , Russia, 05/10/2016

kinetics & reaction network

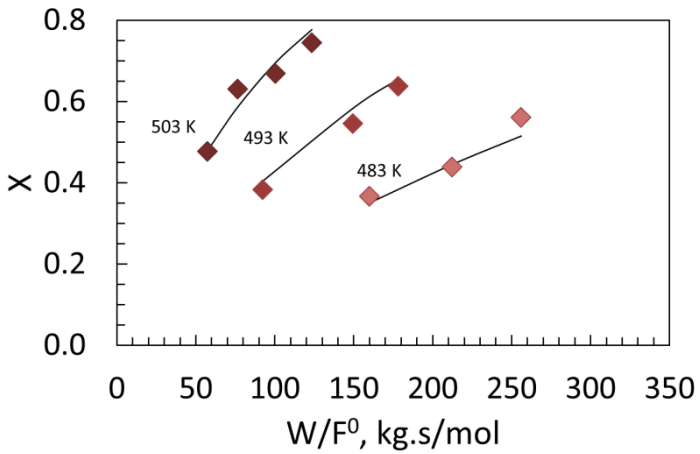
- experimental study on Cu catalyst

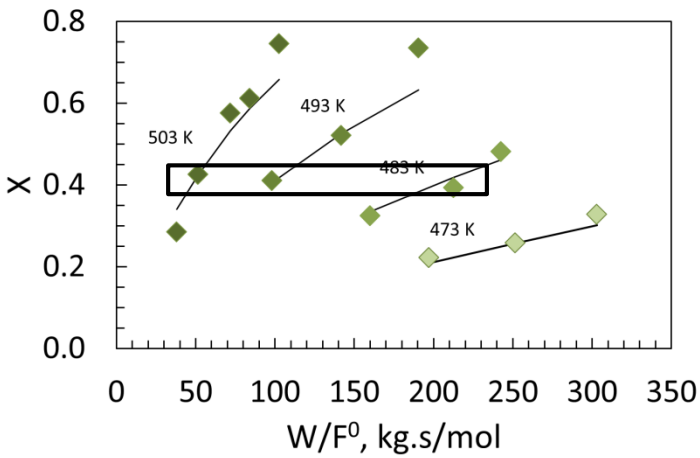


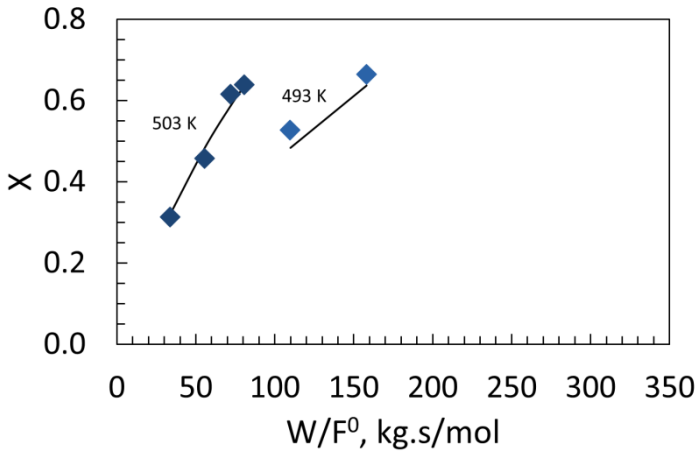
† N. Navidi, J.W. Thybaut, G.B. Marin, Appl. Catal. Gen. 469 (2014) 357–366.

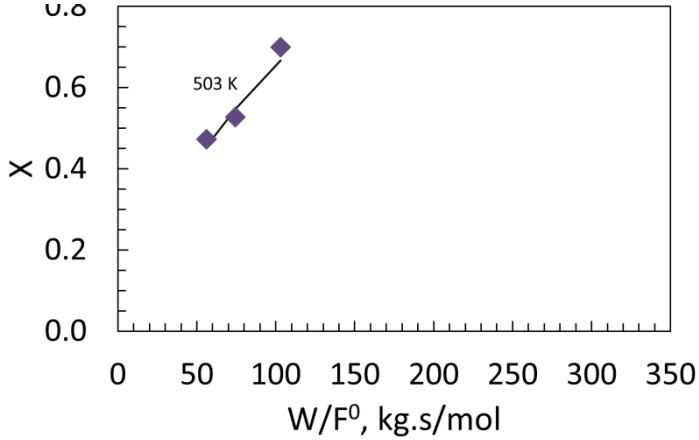
copper based catalysts

Benchmark	Cu1	Cu2	Cu3	Cu4
Cu-A	Cu-AB	Cu-B	Cu-C	0.9Cu-B









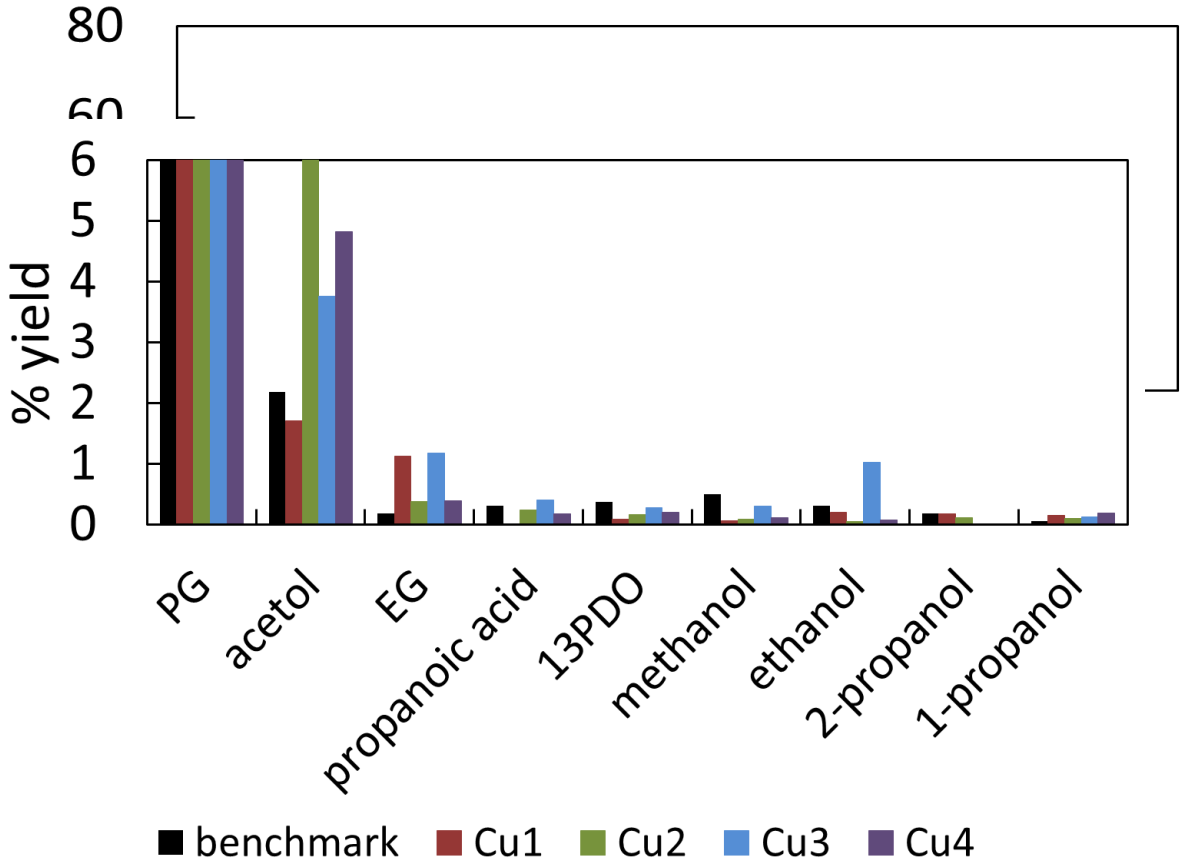
- Similar trends as benchmark for W/F^0 & T

copper based catalysts

Benchmark	Cu1	Cu2	Cu3	Cu4
Cu-A	Cu-AB	Cu-B	Cu-C	0.9Cu-B

@ iso X

- PG yield
- Acetol yield
- Side-product yield



copper based catalysts

Benchmark	Cu1	Cu2	Cu3	Cu4
Cu-A	Cu-AB	Cu-B	Cu-C	0.9Cu-B

@identical operating conditions

- differences activity
- differences stability

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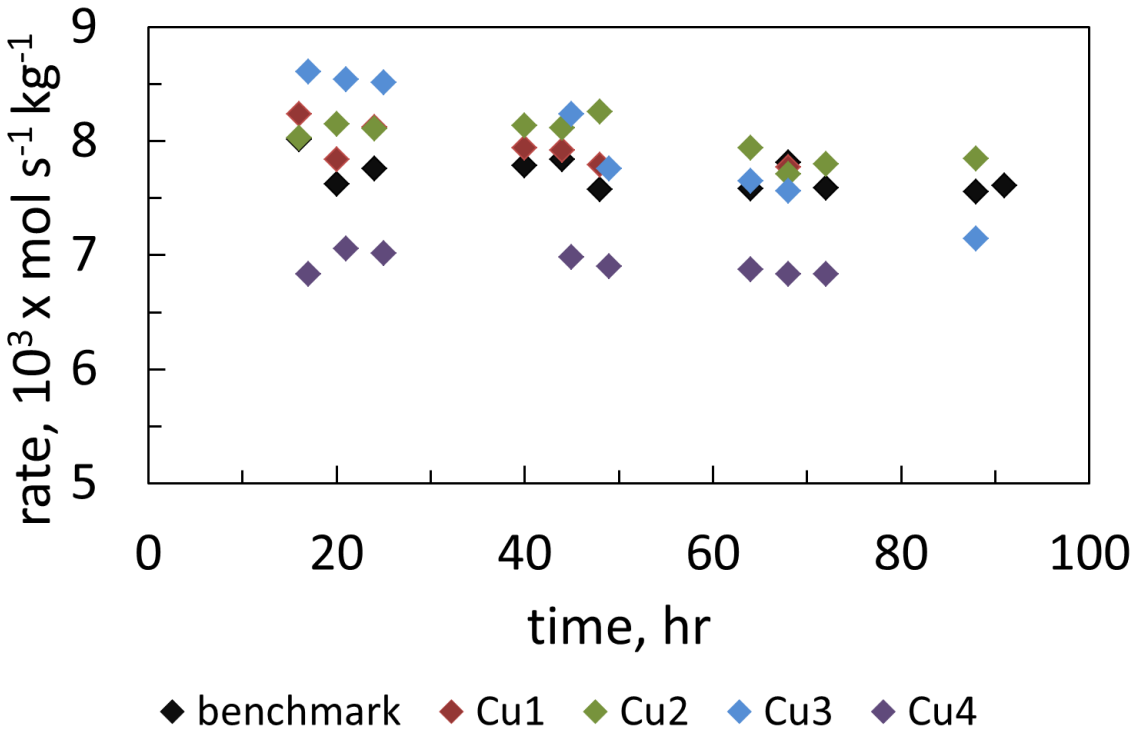
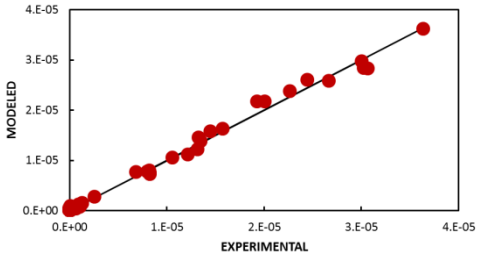
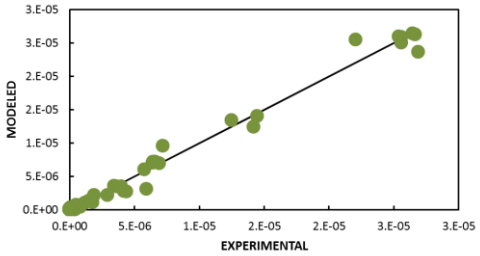
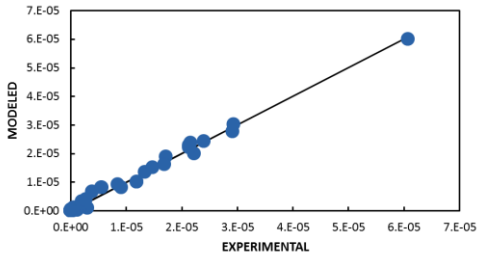
in-adequate metal support interaction

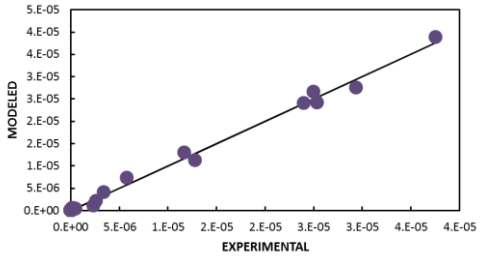


model performance: catalyst descriptors









Rate Coeff		**benchmark**	**Cu1**	**Cu2**	**Cu3**	**Cu4**
	A		Ea			
k_1	10^{15}		84.2			
k_2	10^{13}		59.3			
k_3	10^{12}		86.1			
k_4	10^{14}		100.0			
k_5	10^{13}		87.7			
k_6	10^{13}		87.5			
k_7	10^{14}		94.6			
k_8	10^{12}		116.0			
Eq. const	ΔS^0		$-\Delta H^0$			
K_G	-168		65.70			
K_A	-166	66.4	57.6±0.9	57.9±0.8	57.8±1.3	57.6±1.1
K_{PG}	-143	48.1	53.4±0.3	54.2±0.4	52.8±0.3	54.1±0.4
K_H	-136	55.8	62.5±0.8	59.7±0.6	64.0±0.6	60.8±0.8
K_{H2O}	-154		47.3			
Eq. const			$-\Delta H^0$			
K_{AH}	0		2.4			
Fvalue (F_{tab}: 1.97)			$1.8x10^3$	$2.0x10^3$	$3.8x10^3$	$2.3x10^3$

conclusions

- glycerol hydrogenolysis has been studied on a series of supported Cu catalysts.
- differences in catalyst stability ascribed to differences in metal support interaction leading to sintering.
- bench catalyst derived model capable to reproducing data with all the Cu based catalysts.
- differences in selectivity can be ascribed to differences in hydrogen adsorption.

acknowledgement

The Research leading to this results has received funding from

- IWT
  … the Institute for the Promotion of Innovation through Science and Technology in Flanders (IWT Vlaanderen).”
- i-CaD
  … the European Research Council under the European Union’s Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement n° 615456.”

Thank you